Structural Transformations at the (001) Surface of Oxidized $SrTiO_3$ Studied by the X-ray Surface Diffraction

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Beamline(s): **X14A**

Introduction: $SrTiO_3$ has gained recent attention as a high-**k** dielectric material with unique physical properties. Annealing in an oxygen atmosphere is typically used as a preparation step for producing well-ordered atomically clean $SrTiO_3$ surfaces [1]. Due to the complex defect chemistry and chemical instability this annealing is accompanied by stoichiometry changes in the near surface region and eventually leads to structural transformations [2]. We applied surface X-ray diffraction and CTR scattering to address these changes.

Methods and Materials: Single crystals of $SrTiO_3$(001) were annealed in an O_2 flow in a clean quartz tube at 900, 1000 and 1100°C for 3 hours. An AFM analysis showed the droplet-like features on the surfaces of all samples similar to those reported in [2].

The surface X-ray diffraction was performed at the X14A beamline. The incident X-ray beam was monochromized at 8.0 keV by the double-crystal monochromator, focused horizontally by a sagittally bent second mono-crystal and focused vertically by a mirror.

Results: Radial Q-scans measured from all oxidized $SrTiO_3$ samples at small grazing incident angle revealed a sequence of diffraction peaks (Fig.1). The circular ϕ-scans through these peaks showed weak intensity variations, i.e. the diffracted intensity is concentrated along quasi-powder rings. Such a diffraction pattern originates from the crystalline particles with nearly random in-plane orientation and was associated with the droplets observed by AFM. Analysis based on the available powder diffraction data [3] identified these crystallites as monoclinic TiO. Remarkable changes in specular (00L) CTR intensity were also found indicating significant structural modifications in $SrTiO_3$ surface layer.

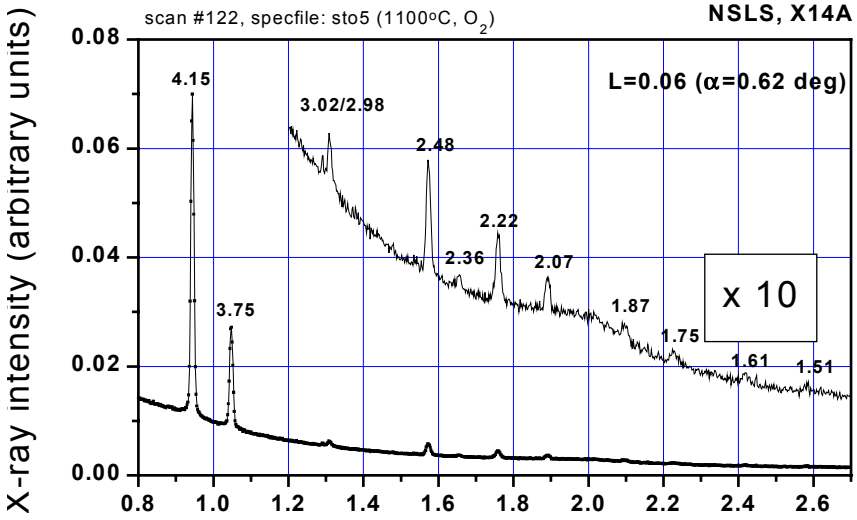

Figure 1. Radial Q-scan at some arbitrary azimuthal angle from the $SrTiO_3$(001) surface oxidized at 1100°C . The incident angle is 0.62 deg. The Q-axis is in reciprocal lattice units for $SrTiO_3$ (a=3.905 Å). Each of the quasi-powder peaks is labeled according to the corresponding d-spacing in Å.

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